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Conformational analysis of 1,3,2-dioxaphospholane and pyrocatehine phosphite with Oc(O)Cf 3 exocyclic substituents

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Abstract

Conformational analysis of 1,3,2-dioxaphospholane-2-yl-2,2,2- trifluoroacetate and 4,5-benz--1,3,2-dioxaphosphole-2-yl-2,2,2-trifluoroacetate was carried out by dipole moment method and quantum chemical calculations (DFT B3LYP/6-31G). © 2013 Copyright Taylor and Francis Group, LLC.

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Keywords

conformational analysis, dipole moments, Heterocyclic organophosphorus compounds, quantum chemical calculations